

# Brueckner approach to the spin-wave gap critical index for the two-layer Heisenberg antiferromagnet

P.V.Shevchenko<sup>a</sup>, O.P.Sushkov

*School of Physics, The University of New South Wales, Sydney 2052, Australia*

(28 September 1998)

We consider the two-layer Heisenberg antiferromagnet near a zero temperature quantum phase transition from a disordered dimer phase to a collinear Neel state. At approaching the transition point the spin-wave gap vanishes as  $\Delta \propto (J_{\perp} - J_{\perp c})^{\nu}$ . To account for strong correlations between the  $S = 1$  elementary excitations we apply the Brueckner diagram approach which gives the critical index  $\nu \approx 0.5$ . We demonstrate also that the linearized in density Brueckner equations give the mean field result  $\nu = 1$ . Finally an expansion of the Brueckner equations in powers of the density, combined with the scaling hypothesis, give  $\nu \approx 0.67$ . This value reasonably agrees with that of the nonlinear  $O(3)$   $\sigma$ -model. Our approach demonstrates that for other quantum spin models the critical index can be different from that in the nonlinear  $\sigma$ -model. We discuss the conditions for this to occur.

PACS codes: 75.10.Jm, 75.30.Kz, 75.50.Ee

keywords: Heisenberg antiferromagnet, spin liquid

There is a significant interest in the physics of quantum phase transitions in  $S = 1/2$  two-dimensional (2D) Heisenberg models in connection with the high- $T_c$  cuprate superconductors. It has been argued by Haldane [1] and Chakravarty, Halperin and Nelson [2] that the phase transition is described by the 2+1-dimensional non-linear  $O(3)$   $\sigma$  model predicting that at approaching the transition point the spin-wave gap vanishes as  $\Delta \sim (J_\perp - J_{\perp c})^\nu$  with critical index  $\nu \approx 0.7$ . Assuming the  $\sigma$ -model description the universal dynamic and static properties of two-dimensional antiferromagnets in the vicinity of a zero-temperature phase transition have been studied in detail by Sachdev, Ye and Chubukov [3,4]. However mapping of the Heisenberg model to the  $\sigma$ -model has been proven only for the one-layer square lattice antiferromagnet which itself does not exhibit a zero temperature quantum phase transition.

In the present work we investigate the two-layer Heisenberg antiferromagnet which has a zero temperature quantum phase transition from a disordered dimer phase to a collinear Neel phase as the dimerization decreases. For this model the numerical results of Singh, Gelfand and Huse [5] and Weihong [6] obtained by series expansions, as well as Monte Carlo calculations performed by Sandvick and Scalapino [7] demonstrate reasonable consistency of the critical index with that in the  $\sigma$ -model. At the same time Sandvik and Vekic [8] using quantum Monte-Carlo simulations have shown that for some other 2D antiferromagnetic models (dimers arranged in ladders and dimers in a staggered pattern) the critical exponents are different from the nonlinear  $\sigma$ -model prediction. In this situation it is very important to analyze the behavior near the critical points by an independent analytical method. Such a method, based on the Brueckner perturbation theory, has been developed in the paper [9]. In the present work we apply it for the calculation of the spin-wave gap critical index in the two-layer Heisenberg antiferromagnet. This method gives an independent calculation of the index for this model, and additionally it allows us to formulate the conditions when one could expect deviations from the  $\sigma$ -model behavior.

We consider the two-layer,  $S = 1/2$ , Heisenberg antiferromagnet described by

$$H = J \sum_{\langle i,j \rangle} (\mathbf{S}_{1i} \mathbf{S}_{1j} + \mathbf{S}_{2i} \mathbf{S}_{2j}) + J_\perp \sum_i \mathbf{S}_{1i} \mathbf{S}_{2i}. \quad (1)$$

The spins  $\mathbf{S}_1$  and  $\mathbf{S}_2$  represent two planes coupled by  $J_\perp$ . Both couplings are antiferromagnetic ( $J, J_\perp > 0$ ) and the first sum runs over nearest neighbors on a square lattice. Considering the “J-terms” in (1) as a perturbation one can introduce the bond operator representation [10,11] and *exactly* map the Hamiltonian (1) to the effective Hamiltonian [9]:

$$H_{eff} = H_2 + H_4 + H_U, \quad (2)$$

$$H_2 = \sum_{\mathbf{k}, \alpha} A_{\mathbf{k}} t_{\mathbf{k}, \alpha}^\dagger t_{\mathbf{k}, \alpha} + \frac{B_{\mathbf{k}}}{2} (t_{\mathbf{k}, \alpha}^\dagger t_{-\mathbf{k}, \alpha}^\dagger + h.c.), \quad (3)$$

$$H_4 = \frac{J}{2} \sum_{\langle i,j \rangle, \alpha, \beta} \{t_{\alpha i}^\dagger t_{\beta j}^\dagger t_{\beta i} t_{\alpha j} - t_{\alpha i}^\dagger t_{\alpha j}^\dagger t_{\beta i} t_{\beta j}\}, \quad (4)$$

$$H_U = U \sum_{i, \alpha, \beta} t_{\alpha i}^\dagger t_{\beta i}^\dagger t_{\beta i} t_{\alpha i}, \quad U \rightarrow \infty, \quad (5)$$

where  $t_{\alpha i}^\dagger$  is the creation operator of the triplet at the bond  $i$  and  $\alpha = x, y, z$  is the polarization of the triplet. The operator  $t_{\mathbf{k}, \alpha}^\dagger$  is the Fourier transform of  $t_{\alpha i}^\dagger$ :  $t_{\mathbf{k}, \alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} t_{\mathbf{r}, \alpha} e^{i(\mathbf{k} + \mathbf{k}_0) \cdot \mathbf{r}}$ . As usual the momentum takes values inside the Brillouin zone  $-\pi < k_x \leq \pi$ ,  $-\pi < k_y \leq \pi$ , but we shift the argument in the Fourier transform by  $\mathbf{k}_0 = (\pi, \pi)$ . In this notation the minimum of the spin-wave dispersion is at  $\mathbf{k} = 0$ . The coefficients are of the form  $A_{\mathbf{k}} = J_\perp + 2J\xi_{\mathbf{k}}$ ,  $B_{\mathbf{k}} = 2J\xi_{\mathbf{k}}$ ,  $\xi_{\mathbf{k}} = -\frac{1}{2}(\cos k_x + \cos k_y)$ . An infinite on-site repulsion between triplets  $H_U$  is introduced to take into account the hard-core constraint  $t_{\alpha i}^\dagger t_{\beta i}^\dagger = 0$  (only one triplet can be excited on a bond). The interaction  $H_U$  gives the dominant contribution to the renormalization of the spin-wave spectrum. It has been demonstrated [9] that in the Brueckner approximation this renormalization is described by the self-energy operator

$$\Sigma(\mathbf{k}, \omega) = \frac{4}{N} \sum_{\mathbf{q}} Z_{\mathbf{q}} v_{\mathbf{q}}^2 \Gamma(\mathbf{k} + \mathbf{q}, \omega - \omega_{\mathbf{q}}), \quad (6)$$

where the scattering amplitude is

$$\Gamma(\mathbf{q}, \omega) = - \left( \frac{1}{N} \sum_{\mathbf{p}} \frac{Z_{\mathbf{p}} Z_{\mathbf{q}-\mathbf{p}} u_{\mathbf{p}}^2 u_{\mathbf{q}-\mathbf{p}}^2}{\omega - \omega_{\mathbf{p}} - \omega_{\mathbf{q}-\mathbf{p}}} \right)^{-1}, \quad (7)$$

and the spin wave spectrum  $\omega_{\mathbf{k}}$ , quasiparticle residue  $Z_{\mathbf{k}}$  and Bogoliubov parameters  $u_{\mathbf{k}}$ ,  $v_{\mathbf{k}}$  are given by the formulas:

$$\omega_{\mathbf{k}} = Z_{\mathbf{k}} \sqrt{\tilde{A}_{\mathbf{k}}^2 - \tilde{B}_{\mathbf{k}}^2}, \quad (8)$$

$$\tilde{A}_{\mathbf{k}} = J_\perp + 2J\xi_{\mathbf{k}} + \Sigma(\mathbf{k}, 0) + 4J\xi_{\mathbf{k}} \sum_{\mathbf{q}} \xi_{\mathbf{q}} Z_{\mathbf{q}} v_{\mathbf{q}}^2, \quad (9)$$

$$\tilde{B}_{\mathbf{k}} = 2J\xi_{\mathbf{k}} - 4J\xi_{\mathbf{k}} \sum_{\mathbf{q}} \xi_{\mathbf{q}} Z_{\mathbf{q}} u_{\mathbf{q}} v_{\mathbf{q}},$$

$$Z_{\mathbf{k}} = \left( 1 - \frac{\partial \Sigma}{\partial \omega} \bigg|_{\omega=0} \right)^{-1}, \quad (10)$$

$$u_{\mathbf{k}}^2, v_{\mathbf{k}}^2 = \frac{Z_{\mathbf{k}} \tilde{A}_{\mathbf{k}}}{2\omega_{\mathbf{k}}} \pm \frac{1}{2}.$$

These equations take also into account the quartic interaction (4) in one-loop approximation. In order to find spectrum, equations (6,7,8,9,10) have to be solved self-consistently for  $\Sigma(\mathbf{k}, 0)$  and  $Z_{\mathbf{k}}$ . The plot of the spin-wave gap  $\Delta$  versus  $J_{\perp}/J$  is presented in Fig.1. In the same figure we present results from the papers [6,9] obtained by the dimer series expansions.

Close to the critical point ( $\Delta \ll J$ ) and for small momenta ( $k \ll 1$ ) the dispersion can be represented as

$$\omega_{\mathbf{k}} \approx \sqrt{\Delta^2 + c^2 k^2}, \quad (11)$$

where  $c = 1.85J$  is the spin-wave velocity [6,9,12]. To find the critical index let us write eq. (8) at the point  $\mathbf{k} = 0$

$$\Delta^2 = Z_0^2(\tilde{A}_0^2 - \tilde{B}_0^2). \quad (12)$$

It is convenient to introduce the values of  $\tilde{A}_0$  and  $\tilde{B}_0$  at the critical point:  $\tilde{A}_{0c} = -\tilde{B}_{0c}$ . Let us vary  $J_{\perp}$  keeping  $J$  fixed, and let us introduce the deviation from the critical point  $\delta J_{\perp} = J_{\perp} - J_{\perp c}$ . Considering  $\delta J_{\perp}$  and  $\Delta$  as independent variables and using eqs. (9,10,11) we find the variations of  $\tilde{A}_0$  and  $\tilde{B}_0$ :

$$\tilde{A}_0 = \tilde{A}_{0c} + \delta J_{\perp} + \delta \Sigma(0, 0) - \frac{Z_0 J \tilde{A}_{0c}}{\pi c^2} \Delta, \quad (13)$$

$$\tilde{B}_0 = \tilde{B}_{0c} + \frac{Z_0 J \tilde{A}_{0c}}{\pi c^2} \Delta.$$

To find the variation of the self-energy notice that according to eq. (7)  $\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) \propto q$  at  $\Delta/c \sim q \ll 1$ . Therefore from eq. (6) we find

$$\delta \Sigma(0, 0) \propto \sum_{\mathbf{q}} q \delta v_{\mathbf{q}}^2 \propto \Delta^2 \ln \frac{J}{\Delta}. \quad (14)$$

Terms linear in  $\Delta$  are canceled out after substitution of (13) and (14) into eq. (12), and neglecting logarithmic dependence we find

$$\Delta \propto \sqrt{\delta J_{\perp}}. \quad (15)$$

Thus the critical index in the Brueckner approximation is  $\nu = 0.5$ . It is known from nuclear and atomic physics [13] that the Brueckner approximation usually works pretty well even in systems with high density, but parametrically it is justified only at the low density limit. In essence it is the dilute gas approximation. It has been demonstrated [9] that for the model under consideration the actual small parameter is  $n_b \ln(J/\Delta)$ , where  $n_b \approx 0.1$  is density of the triplet excitations. It is clear that when the gap is very small this parameter is becoming large and the gas approximation can fail. To analyze the situation numerically we plot in the Fig.2 the functions

$$f_1(x) = \left( \frac{d \ln(\Delta/J)}{dx} \right)^{-1}, \quad (16)$$

$$f_2(x) = - \left( \frac{d \ln(\Delta/J)}{dx} \right)^2 \bigg/ \frac{d^2 \ln(\Delta/J)}{d^2 x},$$

where  $x = J_{\perp}/J$  and  $\Delta$  is found from eqs. (6,7,8,9,10). For pure scaling behavior [ $\Delta \propto (\delta J_{\perp})^{\nu}$ ] the function  $f_1(x)$  is linear and the function  $f_2$  gives the index:  $f_2(x) = \nu$ . Keeping in mind that when the gap is small ( $\ln(J/\Delta) \gg 1$ ) our approximation is not justified, we conclude from the plot of  $f_2$  that the estimate of the critical index is  $\nu \in [0.6, 0.75]$  or

$$\nu \approx 0.67 \pm 0.07. \quad (17)$$

Another way to look at the critical index is to expand the Brueckner equations in powers of the density  $n_b$ . In the leading approximation  $Z_{\mathbf{q}} = u_{\mathbf{q}} = 1$  and therefore the vertex (7) takes the form

$$\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) = \left( \int \frac{d^2 \mathbf{p}}{(2\pi)^2} \frac{1}{\omega_{\mathbf{q}} + \omega_{\mathbf{p}} + \omega_{\mathbf{p}-\mathbf{q}}} \right)^{-1}. \quad (18)$$

In contrast to (7) it does not vanish at  $q \rightarrow 0$ . Let us denote  $\Gamma(0, 0) = \Gamma_c$ . The last terms in the equations (13) are due to the quartic interaction  $H_4$  (4). This interaction is relatively small and therefore we neglect these terms. Below we prove that they are really small. So instead of eqs. (13) we have

$$\begin{aligned} \tilde{A}_0 &= \tilde{A}_{0c} + \delta J_{\perp} + \delta \Sigma(0, 0) \\ \tilde{B}_0 &= \tilde{B}_{0c}. \end{aligned} \quad (19)$$

If we substitute this into eq.(12) and neglect terms quadratic in  $\Delta$  we find that variation of  $\tilde{A}_0$  must vanish

$$\delta \tilde{A}_0 = \delta J_{\perp} + \delta \Sigma(0, 0) = 0. \quad (20)$$

The variation of the self-energy should be found from eq. (6)

$$\delta \Sigma(0, 0) = 4 \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) \delta v_{\mathbf{q}}^2 + 4 \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \delta \Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) v_{\mathbf{q}}^2. \quad (21)$$

The main contribution to the first integral in this formula comes from small momenta ( $q \sim \Delta/c \ll 1$ ) since

$$\delta v_{\mathbf{q}}^2 = \frac{1}{2} \left\{ \frac{\delta \tilde{A}_{\mathbf{q}}}{\omega_{\mathbf{q}}} + \tilde{A}_{\mathbf{q}} \delta \left( \frac{1}{\omega_{\mathbf{q}}} \right) \right\} \approx - \frac{\tilde{A}_{0c} \Delta^2}{4(\Delta^2 + c^2 q^2)^{3/2}}. \quad (22)$$

The variation of  $\tilde{A}$  in this formula vanishes according to eq. (20). Then the integral can be easily evaluated and the result is  $-\Gamma_c \tilde{A}_{0c} \Delta / \pi c^2$ . The main contribution to the second integral in (21) comes from large momenta ( $q \sim 1$ ) where we can write  $\delta \Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) = \Gamma' \delta J_{\perp}$ . It is obvious from (18) that at  $J_{\perp} \gg J$  the derivative  $\Gamma' = 3$ . However we need this derivative near the critical point where the numerical calculation shows that  $\Gamma' \approx 2.9$  independent of momenta. Altogether the variation (21) can be represented as

$$\delta\Sigma(0,0) \approx -\frac{\Gamma_c \tilde{A}_{0c}}{\pi c^2} \Delta + \frac{4}{3} \Gamma' n_b \delta J_\perp, \quad (23)$$

where  $n_b = 3 \sum_{\mathbf{q}} v_{\mathbf{q}}^2 \approx 0.12$  is the density of spin-wave excitations at the critical point. At this step we can check how small is the neglected quartic interaction term in eqs. (13). The ratio of this term to the “ $\Delta$ -term” in (23) is  $J/\Gamma_c \approx 0.15$ , since  $\Gamma_c \approx 6.3J$ . After substitution of (23) into eq. (20) we find the relation between the gap and  $\delta J_\perp$

$$\Delta \approx \frac{\pi c^2}{\Gamma_c A_{0c}} \left(1 + \frac{4}{3} \Gamma' n_b\right) (J_\perp - J_{\perp c}) \approx 1.1(J_\perp - J_{\perp c}). \quad (24)$$

The coefficient 1.1 corresponds to  $\Gamma_c \approx 6.3J$ ,  $A_{0c} \approx 2.4J$ ,  $c \approx 1.9J$ ,  $\Gamma' \approx 2.9$ , and  $n_b \approx 0.12$  which have been found by numerical solution of the linearized in density eqs. (6,8,9,10). We remind that the linearization means that the vertex is taken from eq. (18) and the residues in (9) are replaced by unity ( $Z_{\mathbf{q}} = 1$ ). The numerical solution also gives  $\Delta(J_\perp)$  shown in Fig.1. The slope at  $J_\perp = J_{\perp c}$  is in perfect agreement with the semianalytical formula (24). Thus the leading term in powers of the density gives the critical exponent  $\nu = 1$ , the same as the mean field approximation.

Now, consider the first correction due to the triplet density  $n_b$ . We will keep only those terms which contain additional  $\ln q$  or  $\ln(\Delta/J)$ , so the parameter is  $n_b \ln(\Delta/J)$ . The  $n_b \ln(\Delta/J)$  terms arise only from expansion of the vertex (7), replacing  $u_{\mathbf{p}}^2 u_{\mathbf{q}-\mathbf{p}}^2 = (1 + v_{\mathbf{p}}^2)(1 + v_{\mathbf{q}-\mathbf{p}}^2) \approx 1 + v_{\mathbf{p}}^2 + v_{\mathbf{q}-\mathbf{p}}^2$  we obtain

$$\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) = \left( \int \frac{d^2 p}{(2\pi)^2} \frac{1 + v_{\mathbf{p}}^2 + v_{\mathbf{q}-\mathbf{p}}^2}{\omega_{\mathbf{q}} + \omega_{\mathbf{p}} + \omega_{\mathbf{q}-\mathbf{p}}} \right)^{-1}. \quad (25)$$

After simple integration one can find that for small  $q$  ( $q \sim \Delta/c \ll 1$ ) the vertex is

$$\Gamma(q, -\omega_q) \approx \Gamma_c + \frac{\Gamma_c^2 \tilde{A}}{4\pi c^2} \ln q. \quad (26)$$

Substitution into (21) gives the variation of the self-energy

$$\delta\Sigma(0,0) \approx -\frac{\Gamma_c \tilde{A}_{0c}}{\pi c^2} \Delta \left(1 + \frac{\Gamma_c \tilde{A}_{0c}}{4\pi c^2} \ln \frac{\Delta}{J}\right) + \frac{4}{3} \Gamma' n_b \delta J_\perp, \quad (27)$$

which together with eq. (20) results in

$$\Delta = \frac{\pi c^2}{\Gamma_c \tilde{A}_{0c}} \left(1 + \frac{4}{3} \Gamma' n_b\right) \delta J_\perp \left(1 - \frac{\Gamma_c \tilde{A}_{0c}}{4\pi c^2} \ln \frac{\delta J_\perp}{J}\right). \quad (28)$$

Let us assume the scaling behavior  $\Delta \propto (\delta J_\perp)^\nu$  with  $\nu = 1 - \beta$ . Expanding this formula in powers of  $\beta$  and comparing with (28) we find

$$\nu = 1 - \frac{\Gamma_c \tilde{A}_{0c}}{4\pi c^2} \approx 0.67, \quad (29)$$

which agrees with the estimate (17) and with the result of the  $\sigma$ -model approach ( $\nu \approx 0.70$  [16]).

In conclusion, using the Bruekner approach for two-layer Heisenberg antiferromagnet we have calculated the spin-wave critical index for the zero temperature quantum phase transition. The result is in reasonable agreement with that of the nonlinear  $O(3)$   $\sigma$ -model. This agreement is due to the relative smallness of the quartic interaction for the model under consideration. In this situation the hard-core constraint is the most important and it is very natural that the result is similar to that of the  $\sigma$ -model. However this situation is not general. There are many models where the quartic interaction is very important. It can even produce bound states of triplet spin waves [14] which effectively change the number of relevant degrees of freedom. In this situation one can expect a very substantial deviation from the simple  $\sigma$ -model. An important example of such a system is the 2D  $J_1 - J_2$  model where the singlet bound state has an extremely low energy [15].

We are very grateful to V. N. Kotov, R. R. P. Singh and Z. Weihong for stimulating discussions. This work was supported by a grant from the Australian Research Council.

- 
- <sup>a</sup> e-mail: pavel@newt.phys.unsw.edu.au
- [1] F.D.M.Haldane, Phys.Rev.Lett. **50**, 1153 (1983)
  - [2] S.Chakravarty, B.I.Halperin, and D.R.Nelson, Phys.Rev.Lett. **60**, 1057 (1988)
  - [3] S.Sachdev, J.Ye, Phys.Rev.Lett. **69**, 2411 (1992)
  - [4] A.V.Chubukov, S.Sachdev, and J.Ye, Phys.Rev.B **49**, 11919 (1994)
  - [5] R.R.P.Singh, M.P.Gelfand, and D.A.Huse, Phys.Rev.Lett. **61**, 2484 (1988)
  - [6] Z.Weihong, Phys.Rev.B **55**, 12267 (1997)
  - [7] A.W.Sandvik and D.J.Scalapino, Phys.Rev.Lett. **72**, 2777 (1994)
  - [8] A.W.Sandvik and M.Vekic, J. of Low Temp.Phys. **99**, 314 (1995)
  - [9] V.N.Kotov, O.Sushkov, Z.Weihong and J.Oitmaa, Phys. Rev. Lett. **80**, 5790 (1998).
  - [10] A. V. Chubukov, JETP Lett. **49**, 129 (1989).
  - [11] S. Sachdev and R. Bhatt, Phys. Rev. B **41**, 9323 (1990).
  - [12] K.Hida, J.Phys.Soc.Jpn **61**, 1013 (1992); M.P.Gelfand, Phys.Rev.B **53**, 11309 (1996)
  - [13] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov and O. P. Sushkov. “Relativistic Quantum Electrodynamics and Weak Interaction Effects in Atoms” AIP conference proceedings, **189**, p 254 (1989). Editors: W. Johnson, P. Mohr, J. Sucher.

- [14] O. P. Sushkov and V. N. Kotov. Phys. Rev. Lett. **81**, 1941 (1998).
- [15] V. N. Kotov, J. Oitmaa, O. Sushkov, and Z. Weihong, work in progress.
- [16] M.Ferer and A.Hamid-Aidinejad, Phys.Rev.B **34**, 6481 (1986), and references cited therein

#### FIGURE CAPTIONS

Fig.1 Triplet gap  $\Delta/J$  as a function of  $x = J_{\perp}/J$ . Solid and dashed lines are the results of the self-consistent solution using the Bruekner approach and the Bruekner equations linearized in density respectively. The dots (with error bars) are estimates obtained by dimer series expansions.

Fig.2 Functions  $f_1(x) = \left[ \frac{d \ln(\Delta/J)}{dx} \right]^{-1}$  and  $f_2(x) = - \left[ \frac{d \ln(\Delta/J)}{dx} \right]^2 / \frac{d^2 \ln(\Delta/J)}{dx^2}$  versus  $x = J_{\perp}/J$  (see text).



